LIST OF REFERENCES CITED BY APPLICANT

(Use several sheets if necessary)

ATTY. DOCKET NO.	APPLICATION NO.
9476-003-999	09/644,937
APPLICANT: Nicholls	
FILING DATE: August 23, 2000	GROUP: ~~2857~~ 1631

U.S. PATENT DOCUMENTS

*EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUBCLASS	FILING DATE IF APPROPRIATE
AM	AA	4,855,931	08/08/89	Saunders	364	499	
	AB	5,025,388	06/18/91	Cramer, III et al.	364	496	
	AC	5,526,281	06/11/96	Chapman et al.	364	496	
	AD	5,703,792	12/30/97	Chapman	364	496	
	AE	6,070,127	05/30/00	Hirono et al.	702	27	
	AF	6,185,506	02/06/01	Cramer et al.	702	19	
AM	AG	6,240,374	05/29/01	Cramer et al.	703	11	

FOREIGN PATENT DOCUMENTS

		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUBCLASS	TRANSLATION YES	TRANSLATION NO

OTHER REFERENCES (*Including Author, Title, Date, Pertinent Pages, Etc.*)

AM	AH	Apaya *et al.*, 1995, "The matching of electrostatic extrema: A useful method in drug design? A study of phosphodiesterase III inhibitors," Journal of Computer-Aided Molecular Design 9:33-43
	AI	Arteca *et al.*, 1988, "Shape group studies of molecular similarity: relative shapes of Van der Waals and electrostatic potential surfaces of nicotinic agonists," J. Mol. Graphics 6:45-53
	AJ	Artymiuk *et al.*, 1992, "Similarity searching in databases of three-dimensional molecules and macromolecules," J. Chem. Inf. Comput. Sci. 32(6):617-630
	AK	Barros *et al.*, "Using the triangle inequality to reduce the number of comparisons required for similarity-based retrieval," *In:* Proceedings of IS&T/SPIE: Storage and Retrieval for Still Image and Video Databases IV, 28 Jan. - 2 Feb., 1996, Vol. 2670, pp. 392-403.
	AL	Bath *et al.*, 1994, "Similarity searching in files of three-dimensional chemical structures: Comparison of fragment-based measures of shape similarity," J. Chem. Inf. Comput. Sci. 34:141-147
	AM	Bradley *et al.*, 1993, "Deducing molecular similarity using voronoi binding sites," J. Chem. Inf. Comput. Sci. 33:750-755
	AN	Carbo *et al.*, 1980, "How similar is a molecule to another? An electron density measure of similarity between two molecular structures," International Journal of Quantum Chemistry XVII:1185-1189
	AO	Ciaccia *et al.*, "M-tree: An efficient access method for similarity search in metric spaces," *In:* Proc. 23rd VLDB Conf., Jarke, M., Carey, M.J., Dittrich, K,R., Lochovsky, F.H., Loucopoulos, P., and Jeusfeld, M.A., eds., Athens, Greece, August 1997, pp. 426-435.
	AP	Cioslowski and Nanyakkara, 1993, "Similarity of atoms in molecules," J. Am. Chem. Soc. 115:11213-11215
	AQ	Clarkson, 1997, "Nearest neighbor queries in metric spaces," Proc. 29th ACM Symp. Theory Comp., pp. 609-617.
AM	AR	Constans *et al.*, 1997, "Toward a global maximization of the molecular similarity function: Superposition of two molecules," J. Comput. Chem. 18(6):826-846

AM	AS	Cramer, III *et al.*, 1974, "Substructural analysis. A novel approach to the problem of drug design," Journal of Medicinal Chemistry 17(5):533-535
	AT	Doman *et al.*, 1996, "Algorithm5: A technique for fuzzy similarity clustering of chemical inventories," J. Chem. Inf. Comput. Sci. 36(6):1195-1204
	AU	Drefahl and Reinhard, 1993, "Similarity-based search and evaluation of environmentally relevant properties for organic compounds in combination with the group contribution approach," J. Chem. Inf. Comput. Sci. 33(6):886-895
	AV	Dughan *et al.*, 1991, "The study of peptide bond isosteres using molecular similarity," Journal of Molecular Structure (Theochem) 235:481-488
	AW	Feustel and Shapiro, 1982, "The nearest neighbor problem in an abstract metric space," *In:* Pattern Recognition Letters 1:125-128.
	AX	Good *et al.*, 1992, "Utilization of Gaussian functions for the rapid evaluation of molecular similarity," J. Chem. Inf. Comput. Sci. 32(3):188-191
	AY	Good *et al.*, 1992, "Similarity screening of molecular data sets," Journal of Computer-Aided Molecular Design 6:513-520
	AZ	Good *et al.*, 1995, "New molecular shape descriptors: Application in database screening," Journal of Computer-Aided Molecular Design 9:1-12
	BA	Grant *et al.*, 1996, "A fast method of molecular shape comparison: A simple application of a Gaussian description of Molecular Shape," Journal of Computational Chemistry 17(14):1653-66
	BB	Greene *et al.*, 1994, "Chemical Function Queries for 3D Database Search," J. Chem. Inf. Comput. Sci. 34:1297-1308
	BC	Grethe and Hounshell, "Similarity Searching in the development of new bioactive compounds . An application," *In:* Chemical Structures 2, Warr, W. A., ed., Springer-Verlag, Heidelberg. 1993. Pages 399-407.
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	BE	Hodgkin and Richards, 1987, "Molecular similarity based on electrostatic potential and electric field," International Journal of Quantum Chemistry: Quantum Biology Symposium 14:105-110
	BF	Hudson *et al.*, 1996, "Parameter based methods for compound selection from chemical databases," Quant. Struct.-Act. Relat. 15:285-289
	BG	Jain *et al.*, 1994, "Compass: Predicting biological activities from molecular surface properties. Performance comparisons on a steroid benchmark," Journal of Medicinal Chemistry 37(15):2315-2327
	BH	Johnson, 1989, "A review and examination of the mathematical spaces underlying molecular similarity analysis," Journal of Mathematical Chemistry 3:117-145
	BI	Kato *et al.*, 1987, "A novel method for superimposing molecules and receptor mapping," Tetrahedron 43(22):5229-5236
	BJ	Martin *et al.*, 1990, "Searching databases of three-dimensional structures," *In:* Reviews of Computational Chemistry, Kipkowitz, K. and Boyd, D.B., eds., Vol. 1, pp. 213-263.
	BK	Mestres *et al.*, 1997, "MIMIC: A molecular-field matching program. Exploiting applicability of molecular similarity approaches," J. Comput. Chem. 18(7):934-954
	BL	Meyer and Richards, 1991, "Similarity of molecular shape," Journal of Computer-Aided Molecular Design 5:427-439
	BM	Mezey, 1987, "The shape of molecular charge distributions: group theory without symmetry," Journal of Computational Chemistry 8(4):462-469
AM	BN	Mezey, 1992, "Shape-similarity measures for molecular bodies: A three-dimensional topological approach to quantitative shape-activity relations," J. Chem. Inf. Comput. Sci. 32(6):650-656

AM	BO	Perry and van Geerestein, 1992, "Database searching on the basis of three-dimensional molecular similarity using the SPERM program," J. Chem. Inf. Comput. Sci. 32(6):607-616
	BP	Petitjean, 1995, "Geometric molecular similarity from volume-based distance minimization: Application to saxitoxin and tetrodotoxin," Journal of Computational Chemistry 16(1):80-90
	BQ	Petitjean, 1996, "Three-dimensional pattern recognition from molecular distance minimization," J. Chem. Inf. Comput. Sci. 36(5):1038-1049
	BR	Petke, 1993, "Cumulative and discrete similarity analysis of electrostatic potentials and fields," Journal of Computational Chemistry 14(8):928-933
	BS	Reynolds *et al.*, 1998, "Lead discovery using stochastic cluster analysis (SCA): A new method for clustering structurally similar compounds," J. Chem. Inf. Comput. Sci. 38(2):305-312
	BT	Richard, 1991, "Quantitative comparison of molecular electrostatic potentials for structure-activity studies," Journal of Computational Chemistry 12(8):959-969
	BU	Sprague and Hoffman, "CATALYST Pharmacophore models and their utility as queries for searching 3D databases," *In:* Computer Assisted Lead Finding and Optimization: Current Tools for Medicinal Chemistry, Van de Waterbeemd, H., Testa, B., Folkers, G., eds., VCHA-Basel, 1997, pp. 223-240
	BV	Thorner *et al.*, 1997, "Similarity searching in files of three-dimensional chemical structures: Representation and searching of molecular electrostatic potentials using field-graphs," Journal of Computer-Aided Molecular Design 11:163-174
	BW	Uhlmann, 1991, "Satisfying general proximity/similarity queries with metric trees," *In:* Information Processing Letters 40(4):175-179.
	BX	Walker *et al.*, 1993, "Shape groups of the electronic isodensity surfaces for small molecules: shapes of 10-electron hydrides," Journal of Computational Chemistry 14(10):1172-1183
AM	BY	Weiser *et al.*, 1999, "Optimization of Gaussian surface calculations and extension to solvent-accesible surface areas," Journal of Computational Chemistry 20(7):688-703

EXAMINER Linda Marschel	**DATE CONSIDERED** 9-6-02

*EXAMINER: Initial if reference considered, whether or not citation is in conformance with **MPEP 609**; Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.